

10/5/9, 93)

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FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
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DICTIONARY FILE UPDATES: 2 FEB 2007 HIGHEST RN 919200-33-2

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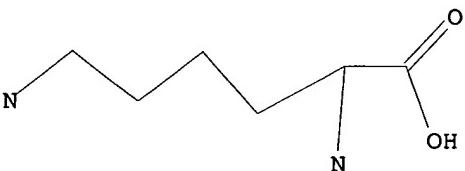
<http://www.cas.org/ONLINE/UG/regprops.html>

\*\*\* YOU HAVE NEW MAIL \*\*\*

=>  
Uploading C:\Program Files\Stnexp\Queries\10519931.str

L1 STRUCTURE uploaded

=> d 11  
L1 HAS NO ANSWERS  
L1 STR



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=> s 11 full  
FULL SEARCH INITIATED 18:58:55 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 447081 TO ITERATE

100.0% PROCESSED 447081 ITERATIONS  
SEARCH TIME: 00.00.04

78138 ANSWERS

L2 78138 SEA SSS FUL L1

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=> file caplus
COST IN U.S. DOLLARS
SINCE FILE          TOTAL
ENTRY           SESSION
FULL ESTIMATED COST      172.10      172.94
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FILE 'CAPLUS' ENTERED AT 18:59:05 ON 04 FEB 2007  
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FILE COVERS 1907 - 4 Feb 2007 VOL 146 ISS 7  
FILE LAST UPDATED: 2 Feb 2007 (20070202/ED)

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\*\*\* YOU HAVE NEW MAIL \*\*\*

```
=> s 12
L3      102262 L2
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=> s 13 and PNA oligomer?
      6248 PNA
      106440 OLIGOMER?
      388 PNA OLIGOMER?
      (PNA(W)OLIGOMER?)
L4      18 L3 AND PNA OLIGOMER?
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=> s 14 and fmoc
      6026 FMOC
L5      6 L4 AND FMOC
```

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=> dup rem 15
PROCESSING COMPLETED FOR L5
L6      6 DUP REM L5 (0 DUPLICATES REMOVED)
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=> d 16 bib abs hitstr 1-6
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```
L6      ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
AN      2006:693745 CAPLUS
DN      145:336301
TI      Modification of guanine residues in PNA-synthesis by PyBOP
AU      Pritz, Stephan; Wolf, Yvonne; Klemm, Clementine; Bienert, Michael
CS      Leibniz-Institute of Molecular Pharmacology, Berlin, 13125, Germany
SO      Tetrahedron Letters (2006), 47(33), 5893-5896
        CODEN: TELEAY; ISSN: 0040-4039
PB      Elsevier B.V.
DT      Journal
LA      English
OS      CASREACT 145:336301
AB      The phosphonium-type coupling reagent PyBOP, when applied to the synthesis
```

of peptide nucleic acid (PNA) oligomers, was found to form O4-phosphonium compds. of the nucleobase guanine which can be converted into C4-modified guanine-derived PNAs by nucleophiles.

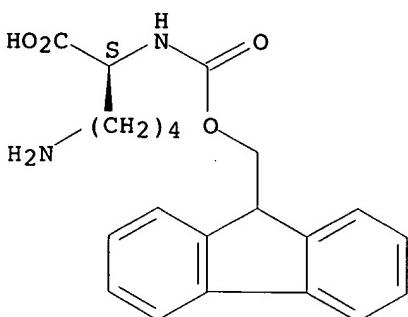
IT 105047-45-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(PNA-synthesis using PyBOP as coupling reagent and determination of guanine-modified byproducts by MS/MS-fragmentation)

RN 105047-45-8 CAPLUS

CN L-Lysine, N2-[(9H-fluoren-9-ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2006:152794 CAPLUS

DN 144:391376

TI An efficient, convenient solid-phase synthesis of amino acid-modified peptide nucleic acid monomers and oligomers

AU Balaji, Baghavathy S.; Gallazzi, Fabio; Jia, Fang; Lewis, Michael R.

CS Department of Veterinary Medicine and Surgery, Molecular Biology Program,  
Department of Radiology, and Nuclear Science and Engineering Institute,  
University of Missouri-Columbia, Columbia, MO, 65211, USA

SO Bioconjugate Chemistry (2006), 17(2), 551-558  
CODEN: BCCHE; ISSN: 1043-1802

PB American Chemical Society

DT Journal

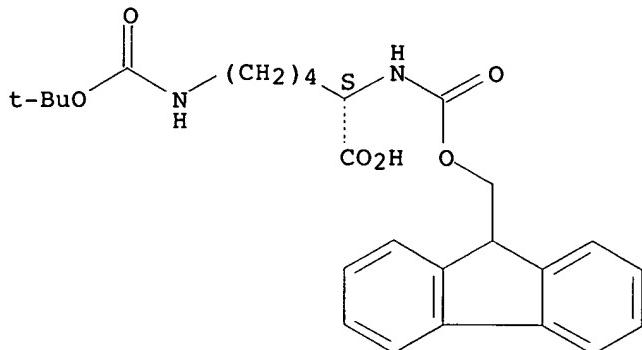
LA English

AB An efficient and highly versatile method for the synthesis of amino acid-modified peptide nucleic acid (PNA) monomers is described. By using solid-phase Fmoc (Fmoc = 9-fluorenylmethoxy carbonyl) techniques, such monomers can be assembled readily in a stepwise manner and obtained in high yield with minimal purification. Protected neutral hydrophilic, acidic, and basic amino acids were coupled to 2-chlorotriptyl chloride resin. Following Fmoc removal, innovative conditions for the key step, reductive alkylation with N-Fmoc -aminoacetaldehyde, were developed to circumvent problems encountered with previously reported methods. Activation and coupling of pyrimidine and purine nucleobases to the resulting secondary amines afforded amino acid-modified PNA monomers. The mild reaction conditions utilized were compatible with sensitive and labile functional groups, such as tert-Bu ethers and tert-Bu esters. PNA monomers were obtained in 36-42% overall yield and very high purity, after cleavage and purification. Using standard solid-phase Fmoc chemical, two of these monomers were incorporated with high coupling efficiency into a variety of modified PNA oligomers, including four tetradecamers designed to target bcl-2 mRNA. Such modified oligomers have the potential to enhance water solubility and cell portability, while maintaining hybridization affinity and promoting favorable biodistribution properties.

IT 71989-26-9

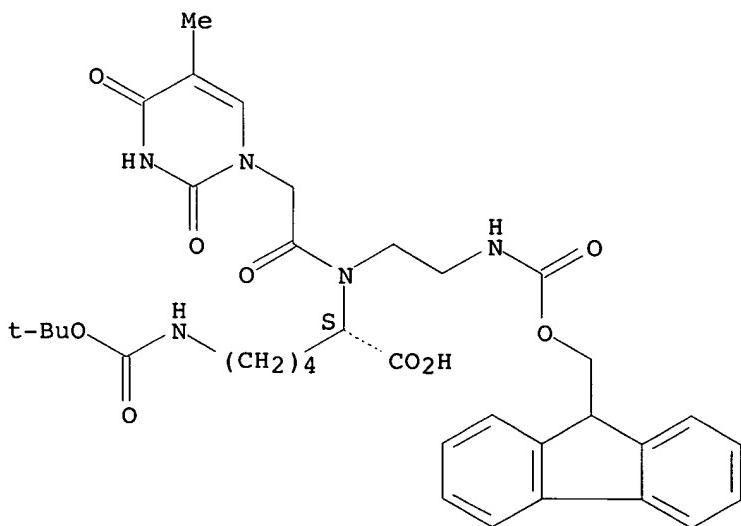
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (solid phase synthesis of peptide nucleic acid monomers and oligomers  
 via reductive alkylation with aminoacetaldehyde as key step)  
 RN 71989-26-9 CAPLUS  
 CN L-Lysine, N6-[(1,1-dimethylethoxy)carbonyl]-N2-[(9H-fluoren-9-  
 ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 882780-21-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (solid phase synthesis of peptide nucleic acid monomers and oligomers  
 via reductive alkylation with aminoacetaldehyde as key step)  
 RN 882780-21-4 CAPLUS  
 CN 13-Oxa-2,5,11-triazapentadecanoic acid, 6-carboxy-5-[(3,4-dihydro-5-methyl-  
 2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-14,14-dimethyl-12-oxo-,  
 1-(9H-fluoren-9-ylmethyl) ester, (6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

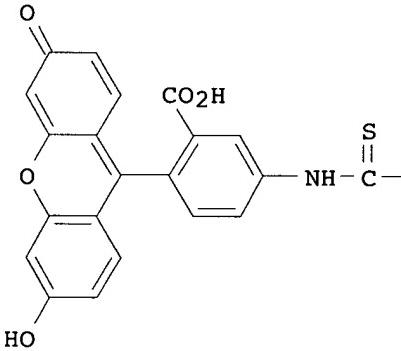
L6 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2004:905902 CAPLUS  
 DN 141:380101  
 TI Novel functional peptide nucleic acid and process for producing the same  
 IN Tonosaki, Madoka; Ikeda, Hisafumi

PA Credia Japan Co., Ltd., Japan  
 SO PCT Int. Appl., 36 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004092377	A1	20041028	WO 2004-JP5392	20040415
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1614750	A1	20060111	EP 2004-727713	20040415
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
	CN 1806045	A	20060719	CN 2004-80016626	20040415
	JP 3800245	B2	20060726	JP 2005-505450	20040415
	US 2006167224	A1	20060727	US 2004-519931	20041230
	IN 2005MN01114	A	20060505	IN 2005-MN1114	20051010
	JP 2006204303	A	20060810	JP 2006-67965	20060313
PRAI	JP 2003-144152	A	20030415		
	JP 2005-505450	A3	20040415		
	WO 2004-JP5392	W	20040415		

GI

Q=



AB In a process for producing a functional PNA oligomer, a PNA monomer unit having protected adenine, guanine, cytosine or thymine is reacted with Boc-Lys(Fmoc)-OH or Fmoc-Lys(Alloc)-OH (Alloc = allyloxycarbonyl) to synthesize a PNA oligomer. Then a functional mol. having a free carboxylic acid is transferred into the above PNA oligomer and the protecting group is deblocked. According to this method having a good cost performance, a functional mol. can be transferred at an extremely high speed. Moreover, this method makes it possible to synthesize the above compound and the Boc-Lys(Fmoc)-OH or Fmoc-Lys(Alloc)-OH serving as a precursor PNA monomer unit. Using this process, a membrane-permeable fluorescent PNA probe R-NH(CH<sub>2</sub>)<sub>6</sub>CO-Lys(R1)-Lys(R1)-Lys(R1)-NH(CH<sub>2</sub>)<sub>6</sub>CO-GCATCCCACTTCTCATCC (I; R = Q; R1 = H-L-Arg-L-Arg-L-Arg) was prepared

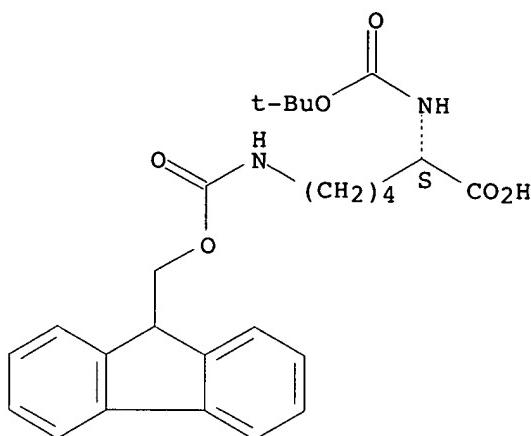
IT 84624-27-1 104669-73-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of novel functional peptide nucleic acid using  $\text{N}\alpha$ -Boc- or  
 $\text{N}\alpha$ -Fmoc-Lys(Fmoc or allyloxycarbonyl)-OH and  
PNA monomers)

RN 84624-27-1 CAPLUS

CN L-Lysine, N2-[ (1,1-dimethylethoxy)carbonyl]-N6-[ (9H-fluoren-9-ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

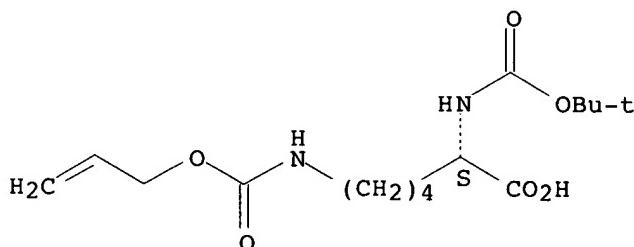
Absolute stereochemistry.



RN 104669-73-0 CAPLUS

CN L-Lysine, N2-[ (1,1-dimethylethoxy)carbonyl]-N6-[ (2-propenyloxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2003:679388 CAPLUS

DN 139:381726

TI Modulation of the Pharmacokinetic Properties of PNA: Preparation of Galactosyl, Mannosyl, Fucosyl, N-Acetylgalactosaminyl, and N-Acetylglucosaminyl Derivatives of Aminoethylglycine Peptide Nucleic Acid Monomers and Their Incorporation into PNA Oligomers

AU Hamzavi, Ramin; Dolle, Frederic; Tavitian, Bertrand; Dahl, Otto; Nielsen, Peter E.

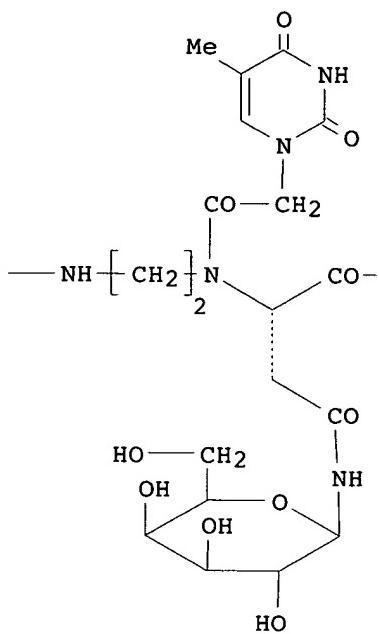
CS Center for Biomolecular Recognition, Department of Medical Biochemistry and Genetics, University of Copenhagen, Copenhagen, DK-2200, Den.

SO Bioconjugate Chemistry (2003), 14(5), 941-954  
CODEN: BCCHE8; ISSN: 1043-1802

PB American Chemical Society

DT Journal

LA English



AB A series of N-(2-aminoethyl)- $\alpha$ -amino acid thymine peptide nucleic acid (PNA) monomers bearing glycosylated side chains in the  $\alpha$ -amino acid position (e.g., I) have been synthesized. These include PNA monomers where glycine has been replaced by serine and threonine (O-glycosylated), derivs. of lysine and nor-alanine (C-glycosylated), and amide derivs. of aspartic acid (N-glycosylated). The Boc and Fmoc derivs. of these monomers were used for incorporation in PNA oligomers. Twelve PNA decamers containing the glycosylated units in one, two, or three positions were prepared, and the thermal stability ( $T_m$ ) of their complexes with a complementary RNA was determined. Incorporation of the glycosyl monomers reduced the duplex stability by 0–6° C per substitution. A cysteine was attached to the amino terminus of eight of the PNA decamers (Cys-CTCATACTCT-NH<sub>2</sub>) for easy conjugation to a [<sup>18</sup>F]radiolabeled N-(4-fluorobenzyl)-2-bromoacetamide. The *in vivo* biodistribution of these PNA oligomers was determined in rat 2 h after i.v. administration. Most of the radioactivity was recovered in the kidneys and in the urine. However, N-acetylgalactosamine (and to a lesser extent galactose and mannose)-modified PNAs were effectively targeting the liver (40-fold over unmodified PNA). Thus, the pharmacodistribution in rats of PNA oligomers can be profoundly changed by glycosylation. These results could be of great significance for PNA drug development, as they should allow modulation and fine-tuning of the pharmacokinetic profile of a drug lead.

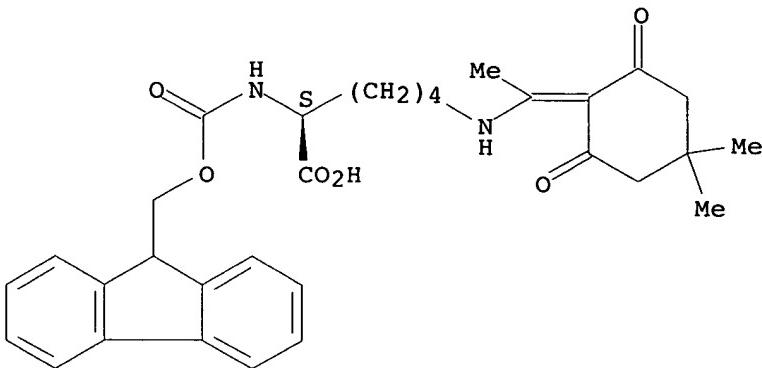
IT 150629-67-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of glycosylated monomers for PNA synthesis and their effect on PNA/RNA hybridization or PNA biodistribution)

RN 150629-67-7 CAPLUS

CN L-Lysine, N6-[1-(4,4-dimethyl-2,6-dioxocyclohexylidene)ethyl]-N2-[(9H-fluoren-9-ylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 612491-20-0P 612491-21-1P 612491-22-2P  
612491-23-3P 612491-24-4P 612491-25-5P

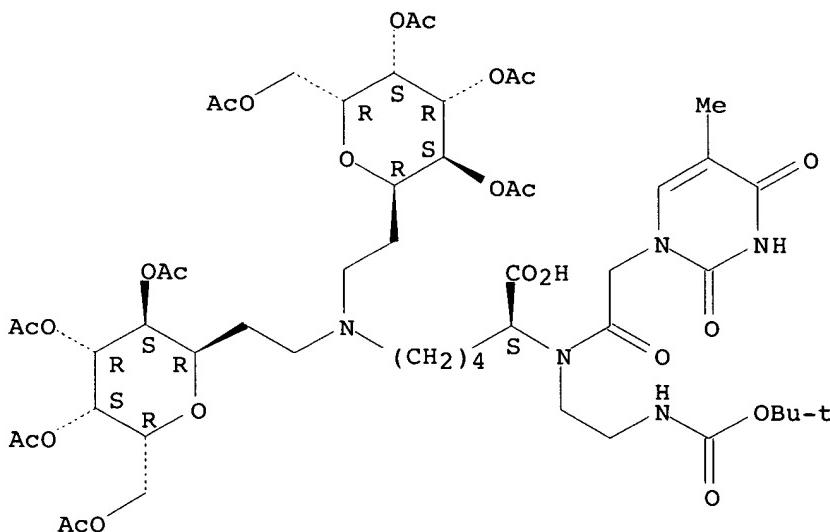
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of glycosylated monomers for PNA synthesis and their effect on PNA/RNA hybridization or PNA biodistribution)

RN 612491-20-0 CAPLUS

CN L-Lysine, N2-[{3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl}acetyl]-N2-[2-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-N6,N6-bis(1,3,4,5-tetra-O-acetyl-2,6-anhydro-7,8-dideoxy-D-glycero-L-galacto-octitol-8-y1)- (9CI)  
(CA INDEX NAME)

## Absolute stereochemistry.

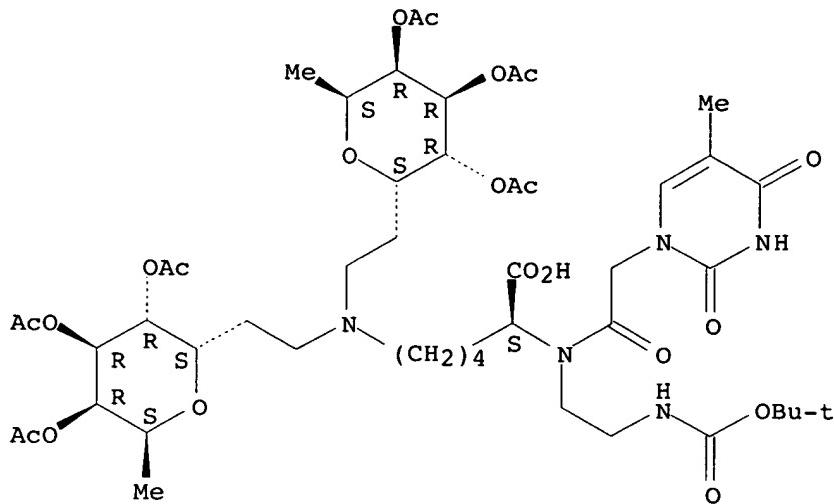


RN 612491-21-1 CAPLUS

CN L-Lysine, N2-[{3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl}acetyl]-N2-[2-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-N6,N6-bis(3,4,5-tri-O-acetyl-2,6-anhydro-1,7,8-trideoxy-L-glycero-D-galacto-octitol-8-yl)- (9CI)  
(CA INDEX NAME)

## Absolute stereochemistry.

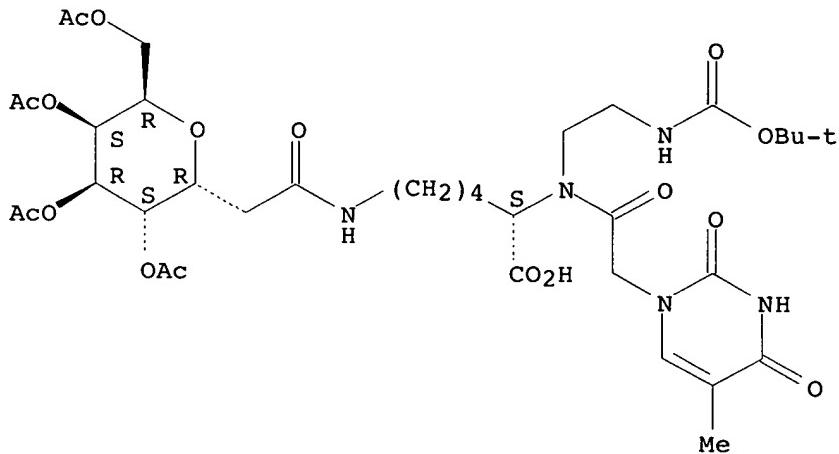
# BEST AVAILABLE COPY



RN 612491-22-2 CAPLUS

CN L-Lysine, N2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-N2-[2-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-N6-(4,5,6,8-tetra-O-acetyl-3,7-anhydro-2-deoxy-D-glycero-L-glucosyloctonoyl)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.



RN 612491-23-3 CAPLUS

CN L-Lysine, N2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-N2-[2-[[9H-fluoren-9-ylmethoxy]carbonyl]amino]ethyl]-N6-(4,5,6,8-tetra-O-acetyl-3,7-anhydro-2-deoxy-D-glycero-L-gluco-octonoyl)- (9CI) (CA INDEX NAME)

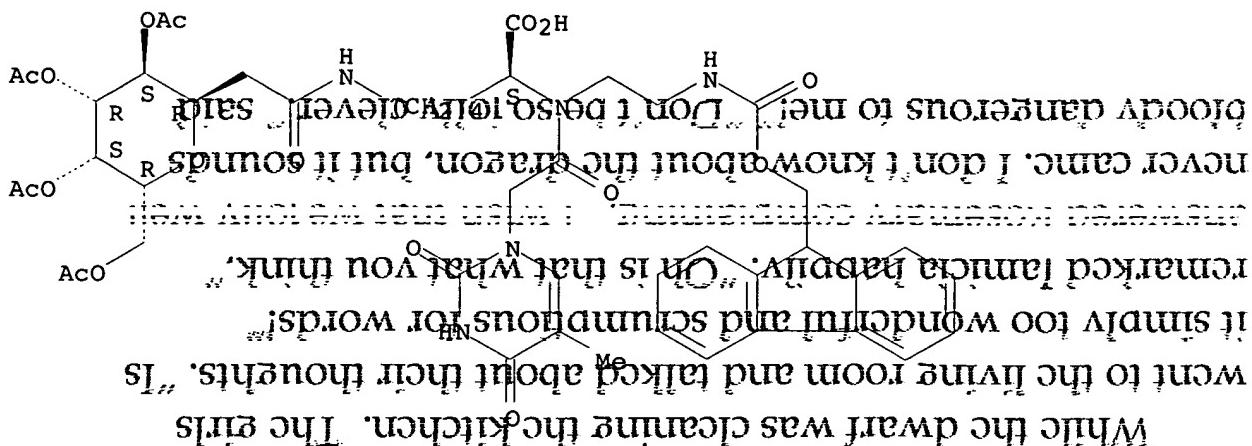
## Absolute stereochemistry.

Food burns better when it's open and in came I understand, I tell

— 1 —

**DEAR TO FRIENDS** **STOOD** **ON** **THE** **STREET** **—** **—** **—**

# **BEST AVAILABLE COPY**



Absolute stereochemistry came to the bart listened, he made no comment until Lamicia came to the bar.

"So where exactly do you come from?" asked Huffigrumma as he cut up his sandwiches. "Well that is sort of hard to explain," said Lamicia, putting down her glass of orange juice. "Well, why don't you get started, and we'll have all morning." And so they did.

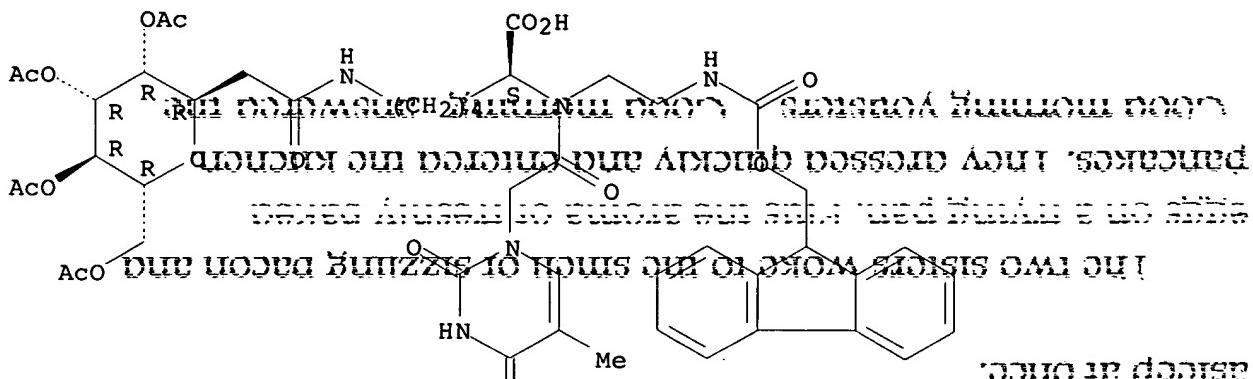
Rosamary exalimed that thev had found the world. After that Lamicia added how thev had found the world.

The crumch of bacon filled the room as they dug into their delicious breakfast. "Umm, delicious" said Rosemary as she cut up her pancake streaming with maple syrup. "Totally" said Lamicia as she crunched on her bacon. "Thank Absolute stereochemistry.

orange juice.

"Sisters, will you tell us if your sister is dishonest ready," said the kind master, knee sat down and ate a

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RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

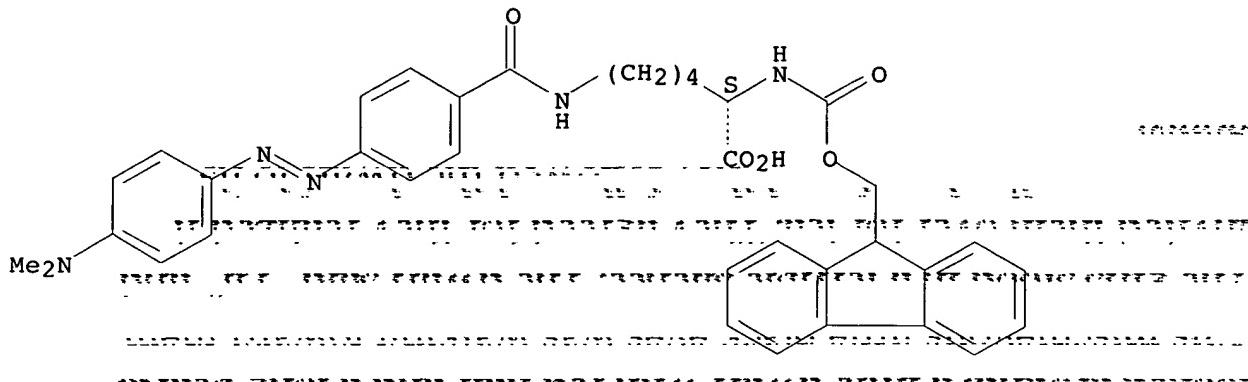
L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN 2001:743877 CAPLUS  
AN 136:295013  
TI Convergent strategies for the attachment of fluorescing reporter groups to  
peptides, nucleic acids in solution and on solid phase  
AU Seitz, Oliver; Kohler, Olaf  
CS MPB für Molekulare Physiologie, Department of Chemical Biology and Institut  
fur Organische Chemie, Universitat Dortmund, Dortmund, 44227, Germany  
SO Chemistry - A European Journal 2001, 17 (18), 5009-5025 CODEN: CEUJED; ISSN: 0947-6539  
PB WILEY-VCH VERLAG GMBH & CO KG  
DT Journal  
LA English  
OS CASREACT 136:295013  
AB The site-selective conjugation of peptide nucleic acids (PNA) with fluorescent reporter groups is essential for the construction of hybridization probes that can report the presence of a particular DNA sequence. This paper describes convergent methods for the solution- and solid-phase synthesis of multiply labeled PNA oligomers. The solid-phase synthesis of protected PNA enabled the selective and efficient attachment of fluorescent labels at the C-terminal end (3' in DNA) which demonstrated that further multiple labeling of protected PNA fragments is feasible. For the conjugation to internal sites, a method is introduced that allows the on-resin synthesis of a PNA fragment by OMM omitting the need to synthesize an entire monomer in solution. Furthermore, it is shown that the application of a highly orthogonal protecting group strategy in combination with chemoselective conjugation reactions provides access to a rapid and automateable solid-phase synthesis of dual-labeled PNA probes. Real-time measurements of nucleic acid hybridization were possible by taking advantage of the fluorescence resonance energy transfer (FRET) between suitably appended fluorophoric groups. Analogously to DNA-based mol. beacons, the dual-labeled PNA probes were only weakly fluorescing in the single-stranded state. Hybridization to a complementary oligonucleotide, however, induced a structural reorganization and conferred a vivid fluorescence enhancement.

IT 146998-27-8  
RL: RET (Reactant); RACT (Reactant or reagent)  
(convergent strategies for attachment of fluorescing reporter groups to  
peptides, nucleic acids in solution and on solid phase)  
RN 146998-27-8 CAPLUS  
CN L-SYNTETIC PEPTIDE CONJUGATE CONSISTING OF A PNA MONOMER WITH A 4-(4-METHOXYCARBONYL)-1-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

**BEST AVAILABLE COPY**

Double bond geometry unknown.



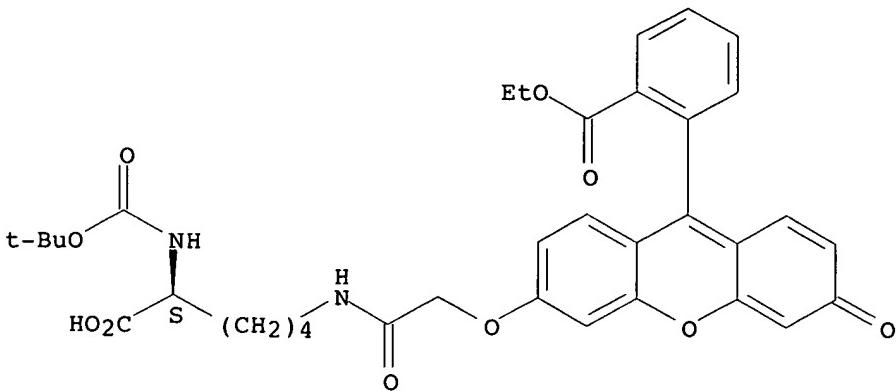
RE.CNT 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER "6" OF "6" CAPLUS COPYRIGHT 2007 ACS on STN  
AN 1997:433584 CAPLUS  
DN 127:81770  
TI Fluorescein-Conjugated Lysine Monomers for Solid Phase Synthesis of Fluorescent Peptides  
AU Lohse, Jesper; Nielsen, Peter E.; Harrit, Niels; Dahl, Otto  
CS Department of Chemistry H. C. Ørsted Institute, University of Copenhagen, Copenhagen, Denmark, Dk-2100, Denmark  
SO Bioconjugate Chemistry (1997), 8(4), 503-509  
CODEN: BCCHE8, ISSN: 1043-1802  
PB American Chemical Society  
DT Journal  
LA English  
AB Fluorescein Et ester was used to prepare the fluorescent mixed ester/ether 6-O-(carboxymethyl)fluorescein Et ester. Conjugation of the latter fluorescein derivative to the ε-amino group of α-N-Boc-L-lysine, via the N-hydroxysuccinimide ester, gave the Boc-protected fluorescein-conjugated lysine monomer. Removal of the Boc group, followed by reaction with Fmoc chloride, gave the Fmoc-protected monomer. These Boc- and Fmoc-protected fluorescein-conjugated lysines were readily incorporated into peptides and PNA oligomers during solid phase synthesis to give fluorescent products. Mass spectroscopy and UV studies showed that the fluorophore remains unchanged during solid phase synthesis. In contrast to fluorescein, the photophysical properties of these derivatives are pH independent from pH 3 to 8, with a molar absorption coefficient,  $\epsilon_{max}$  456, of  $2.2 \pm 104$  M<sup>-1</sup> cm<sup>-1</sup> and fluorescence quantum yield,  $\phi$ , of 0.18.  
IT 191791-24-9 PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
RN (fluorescein-conjugated lysine monomers for solid phase synthesis of fluorescent peptides)  
RN 191791-24-9, CAPLUS  
CN Benzoic acid, 2-[6-[2-[(5-carboxy-5-[(1,1-dimethylethoxy)carbonyl]amino)propyl]amino]-2-oxoethyl]-3-oxo-3H-xanthene-9-yl]-1-ethyl ester, (S)-(9CI) (CA INDEX NAME)

## Absolute stereochemistry.

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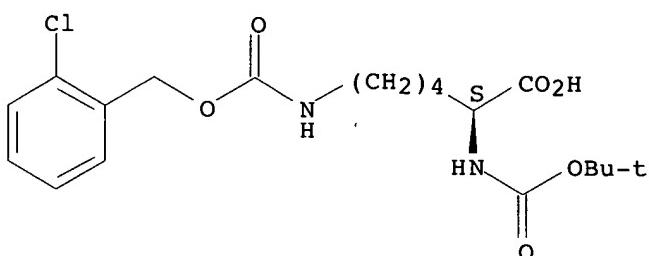
IT 54613-99-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(fluorescein-conjugated lysine monomers for solid phase synthesis of  
fluorescent peptides)

RN 54613-99-9 CAPLUS

CN L-Lysine, N6-[(2-chlorophenyl)methoxy]carbonyl]-N2-[(1,1-dimethylethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 191791-27-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(fluorescein-conjugated lysine monomers for solid phase synthesis of  
fluorescent peptides)

RN 191791-27-2 CAPLUS

CN Benzoic acid, 2-[6-[2-[[5-carboxy-5-[(9H-fluoren-9-yl)methoxy]carbonyl]amino]pentyl]amino]-2-oxoethoxy]-3-oxo-3H-xanthan-9-yl]-, 1-ethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

